

Bis(4-nitrophenyl)phosphoric acid

Other names:	Phosphoric acid, bis(4-nitrophenyl) ester p-Nitrophenyl monohydrogen phosphate Bis(p-nitrophenyl) phosphate Bis(4-nitrophenyl) phosphate BNPP Di-p-nitrophenyl phosphate Phosphoric acid bis(p-nitrophenyl ester) Phenol, p-nitro-, hydrogen phosphate Phosphorsaeure-bis-(p-nitro-phenylester) NSC 59824 bis(4-nitrophenyl) hydrogen phosphate
Inchi:	InChI=1S/C12H9N2O8P/c15-13(16)9-1-5-11(6-2-9)21-23(19,20)22-12-7-3-10(4-8-12)14(
InchiKey:	MHSVUSZEHNVFKW-UHFFFAOYSA-N
Formula:	C12H9N2O8P
SMILES:	O=[N+]([O-])c1ccc(OP(=O)(O)Oc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]:	340.18
CAS:	645-15-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.35		Crippen Method
logp	3.061		Crippen Method
mcvol	211.200	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C645158&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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